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3,4,5-Trimethoxyphenol

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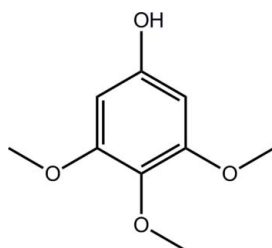
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}–\text{C}) = 0.002$ Å; R factor = 0.051; wR factor = 0.123; data-to-parameter ratio = 13.4.

The asymmetric unit of the title compound, $\text{C}_9\text{H}_{12}\text{O}_4$, consists of two crystallographically independent molecules with similar conformations: essentially planar [r.m.s deviations for $\text{C}_6\text{O}_4 = 0.0057$ and 0.0137 Å] except for the central methoxy-methyl group [C–C–O–C torsion angles = 83.3 (2) and 83.9 (2)°]. In the crystal, O–H...O hydrogen bonds link the molecules, generating supramolecular chains along the b axis. The three-dimensional crystal structure is stabilized by C–H...O and C–H... π interactions.

Related literature

For background information on the energetics and anti-oxidant potential of phenolic compounds, see: Matos *et al.* (2008); Gong *et al.* (2009).



Experimental

Crystal data

$\text{C}_9\text{H}_{12}\text{O}_4$
 $M_r = 184.19$
 Monoclinic, $P2_1/c$
 $a = 15.355$ (3) Å
 $b = 11.139$ (2) Å

$c = 11.546$ (2) Å
 $\beta = 111.38$ (3)°
 $V = 1839.0$ (6) Å³
 $Z = 8$
 Mo $K\alpha$ radiation

$\mu = 0.11$ mm^{−1}
 $T = 296$ K

$0.20 \times 0.15 \times 0.10$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.981$, $T_{\max} = 0.990$
 16747 measured reflections
 3257 independent reflections
 2957 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.123$
 $S = 1.05$
 3257 reflections
 243 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.12$ e Å^{−3}
 $\Delta\rho_{\min} = -0.16$ e Å^{−3}

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C1–C3, C5, C7, C9 and C10–C12, C14, C16, C18 benzene rings, respectively.

$D–H \cdots A$	$D–H$	$H \cdots A$	$D \cdots A$	$D–H \cdots A$
O5–H5...O7 ⁱ	0.82	1.93	2.7484 (18)	179
O1–H1...O3 ⁱⁱ	0.82	1.90	2.7204 (17)	175
C6–H6A...O1 ⁱⁱⁱ	0.96	2.57	3.256 (3)	129
C15–H15A...O5 ^{iv}	0.96	2.59	3.270 (3)	128
C4–H4B...Cg1 ^v	0.96	2.86	3.777 (2)	160
C17–H17B...Cg2 ^{vi}	0.96	2.85	3.736 (2)	154
C13–H13B...O1 ^{vii}	0.96	2.49	3.303 (3)	142

Symmetry codes: (i) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $-x, -y + 2, -z$; (v) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (vi) $x, -y + \frac{1}{2}, z - \frac{3}{2}$; (vii) $x, -y + \frac{3}{2}, z + \frac{1}{2}$.

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5160).

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supplementary materials

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3,4,5-Trimethoxyphenol

Xiao-Chuan Jia, Jing Li, Zhi-Rui Yu, Hui Zhang and Lei Zhou

Comment

The study of the energetics of phenolic compounds (Matos *et al.*, 2008) has considerable practical interest since this class of chemical compound includes a large number of synthetic and naturally occurring antioxidants. They inhibit the oxidation of materials of both commercial and biological importance. This antioxidant function is due to the ability of phenols to trap the peroxy radicals *via* the hydrogen transfer reaction (Gong *et al.*, 2009). In order to expand this field, we now report the structure of the title compound.

The molecule of the title compound (Fig. 1), consists of two crystallographically independent molecules, A and B, with similar conformations. All O-atoms in both molecules are coplanar with the benzene rings they are attached to, and the mean r.s.m in molecules A and B are 0.0057 and 0.0137 Å, respectively.

In the crystal, it is worth mentioning that strong intermolecular O—H \cdots O hydrogen bonds link molecules A and B to generate a one dimensional chain (Fig. 2 and Table 1) along the *b* axis. These are connected into a supramolecular layer in the *bc* plane by C—H \cdots O and C-H $\cdots\pi$ interactions (Table 1). The layers are connected into a three-dimensional crystal structure by C—H \cdots O hydrogen bonds (Table 2) involving the C13 and O1 atoms (Table 1).

Experimental

3,4,5-Trimethoxyphenol was obtained commercially from Aldrich Chemical Co. Single crystals suitable for X-ray diffraction were obtained by recrystallizing the crude product from its chloroform solution by slow evaporation at room temperature over a period of seven days.

Refinement

All H atoms were placed in idealized positions (C—H = 0.93–0.96 Å, O—H = 0.82 Å) and refined as riding atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Computing details

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

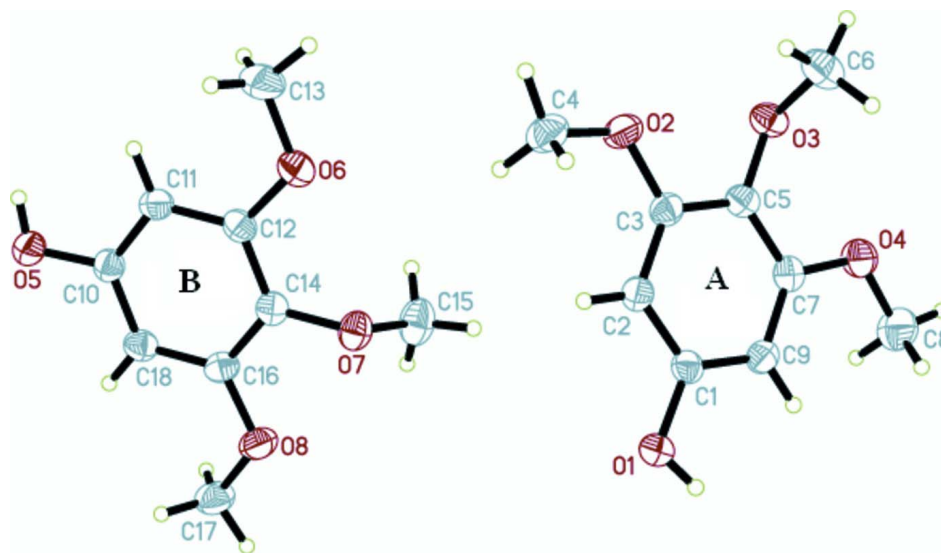


Figure 1

The molecular structure of the title compound, with displacement ellipsoids at the 30% probability level.

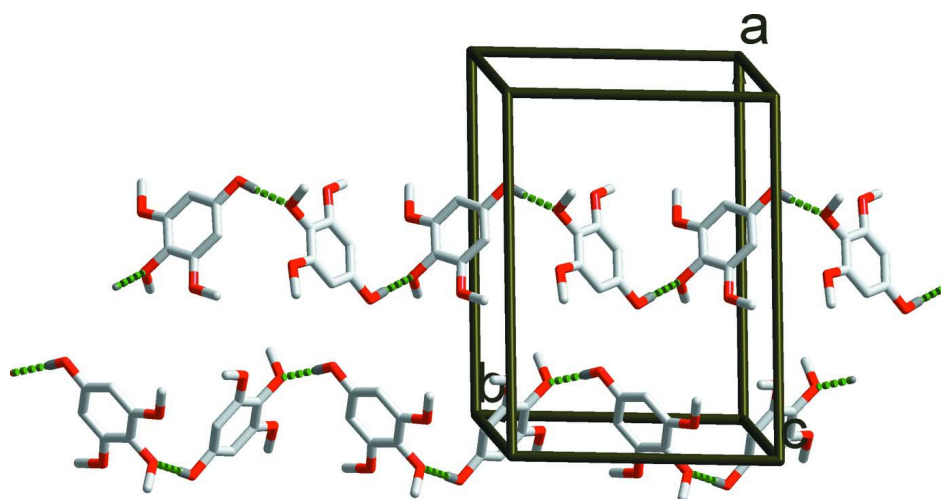


Figure 2

A portion of the unit cell contents highlighting the chain structure of the title compound, linked *via* O—H...O hydrogen bonds (dashed lines). H atoms have been omitted for clarity, except for those involved in hydrogen-bonded interactions.

3,4,5-Trimethoxyphenol

Crystal data

$C_9H_{12}O_4$

$M_r = 184.19$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 15.355\ (3)\ \text{\AA}$

$b = 11.139\ (2)\ \text{\AA}$

$c = 11.546\ (2)\ \text{\AA}$

$\beta = 111.38\ (3)^\circ$

$V = 1839.0\ (6)\ \text{\AA}^3$

$Z = 8$

$F(000) = 784$

$D_x = 1.331\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5944 reflections

$\theta = 3.3\text{--}25.4^\circ$

$\mu = 0.11\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Block, colourless

$0.20 \times 0.15 \times 0.10\ \text{mm}$

Data collection

Bruker SMART CCD area-detector	16747 measured reflections
diffractometer	3257 independent reflections
Radiation source: fine-focus sealed tube	2957 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\text{int}} = 0.025$
φ and ω scans	$\theta_{\text{max}} = 25.1^\circ$, $\theta_{\text{min}} = 3.3^\circ$
Absorption correction: multi-scan	$h = -18 \rightarrow 17$
(<i>SADABS</i> ; Sheldrick, 1996)	$k = -13 \rightarrow 13$
$T_{\text{min}} = 0.981$, $T_{\text{max}} = 0.990$	$l = -11 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.123$	$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 0.3972P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
3257 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
243 parameters	$\Delta\rho_{\text{max}} = 0.12 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.16 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F , and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.33376 (8)	0.41617 (11)	0.19861 (12)	0.0525 (3)
H1	0.3521	0.3629	0.1642	0.079*
O4	0.64034 (9)	0.58079 (12)	0.27042 (13)	0.0602 (4)
O3	0.61501 (8)	0.74092 (10)	0.42789 (11)	0.0509 (3)
C2	0.39182 (12)	0.57694 (14)	0.33613 (15)	0.0445 (4)
H2	0.3366	0.5772	0.3520	0.053*
C3	0.46239 (12)	0.65836 (14)	0.39471 (15)	0.0443 (4)
C5	0.54480 (11)	0.65824 (14)	0.37034 (15)	0.0443 (4)
C7	0.55643 (11)	0.57554 (15)	0.28722 (15)	0.0447 (4)
O2	0.45748 (9)	0.74281 (11)	0.47812 (13)	0.0579 (4)
C9	0.48632 (11)	0.49346 (15)	0.22769 (15)	0.0452 (4)
H9	0.4938	0.4384	0.1715	0.054*
C1	0.40488 (11)	0.49505 (14)	0.25354 (15)	0.0426 (4)
C8	0.64850 (16)	0.5093 (2)	0.1731 (2)	0.0805 (7)
H8A	0.6423	0.4261	0.1903	0.121*
H8B	0.7085	0.5225	0.1673	0.121*
H8C	0.6002	0.5309	0.0958	0.121*

C6	0.67555 (14)	0.7061 (2)	0.55005 (19)	0.0676 (6)
H6A	0.6420	0.7098	0.6057	0.101*
H6B	0.7281	0.7596	0.5786	0.101*
H6C	0.6972	0.6256	0.5478	0.101*
C4	0.38077 (15)	0.73582 (19)	0.5198 (2)	0.0644 (5)
H4A	0.3235	0.7519	0.4514	0.097*
H4B	0.3890	0.7940	0.5843	0.097*
H4C	0.3782	0.6568	0.5517	0.097*
O7	0.11271 (9)	0.75191 (10)	0.18255 (12)	0.0519 (3)
O5	−0.16694 (8)	1.08198 (11)	0.13218 (12)	0.0557 (3)
H5	−0.1501	1.1323	0.1878	0.084*
O6	0.13740 (8)	0.91453 (12)	0.36143 (12)	0.0587 (4)
C16	−0.03779 (12)	0.83857 (15)	0.06267 (15)	0.0462 (4)
C12	0.05455 (11)	0.92090 (15)	0.26236 (15)	0.0440 (4)
C18	−0.10754 (12)	0.92213 (15)	0.05119 (16)	0.0479 (4)
H18	−0.1617	0.9235	−0.0197	0.058*
C14	0.04348 (11)	0.83728 (14)	0.16863 (15)	0.0439 (4)
C11	−0.01507 (11)	1.00391 (15)	0.25244 (15)	0.0456 (4)
H11	−0.0079	1.0590	0.3158	0.055*
O8	−0.04248 (9)	0.75347 (11)	−0.02475 (12)	0.0606 (4)
C10	−0.09552 (11)	1.00336 (15)	0.14650 (16)	0.0450 (4)
C17	−0.11899 (15)	0.75973 (19)	−0.14040 (19)	0.0659 (6)
H17A	−0.1765	0.7496	−0.1266	0.099*
H17B	−0.1131	0.6974	−0.1945	0.099*
H17C	−0.1190	0.8365	−0.1782	0.099*
C15	0.17645 (16)	0.7822 (2)	0.1232 (2)	0.0735 (6)
H15A	0.1450	0.7779	0.0346	0.110*
H15B	0.2279	0.7268	0.1487	0.110*
H15C	0.1994	0.8622	0.1463	0.110*
C13	0.14821 (16)	0.9927 (2)	0.46273 (19)	0.0749 (6)
H13A	0.1435	1.0744	0.4348	0.112*
H13B	0.2084	0.9798	0.5267	0.112*
H13C	0.1001	0.9766	0.4953	0.112*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0433 (6)	0.0543 (8)	0.0560 (7)	−0.0037 (5)	0.0135 (6)	−0.0136 (6)
O4	0.0501 (7)	0.0696 (9)	0.0688 (9)	−0.0055 (6)	0.0311 (7)	−0.0059 (7)
O3	0.0527 (7)	0.0453 (7)	0.0509 (7)	−0.0101 (5)	0.0143 (6)	0.0044 (5)
C2	0.0429 (9)	0.0426 (9)	0.0496 (10)	0.0027 (7)	0.0186 (8)	0.0017 (7)
C3	0.0492 (9)	0.0375 (9)	0.0460 (9)	0.0017 (7)	0.0172 (7)	0.0010 (7)
C5	0.0463 (9)	0.0387 (9)	0.0454 (9)	−0.0035 (7)	0.0139 (7)	0.0049 (7)
C7	0.0438 (9)	0.0461 (10)	0.0458 (9)	0.0033 (7)	0.0182 (7)	0.0074 (7)
O2	0.0614 (8)	0.0503 (7)	0.0698 (9)	−0.0090 (6)	0.0330 (7)	−0.0185 (6)
C9	0.0490 (9)	0.0439 (9)	0.0427 (9)	0.0047 (8)	0.0167 (7)	−0.0002 (7)
C1	0.0406 (8)	0.0418 (9)	0.0408 (8)	0.0029 (7)	0.0092 (7)	0.0035 (7)
C8	0.0706 (14)	0.0924 (17)	0.0975 (17)	−0.0050 (12)	0.0533 (13)	−0.0198 (14)
C6	0.0596 (12)	0.0693 (13)	0.0594 (12)	−0.0081 (10)	0.0047 (10)	0.0066 (10)
C4	0.0720 (13)	0.0632 (12)	0.0698 (13)	−0.0076 (10)	0.0399 (11)	−0.0177 (10)

O7	0.0555 (7)	0.0461 (7)	0.0579 (8)	0.0084 (5)	0.0253 (6)	0.0097 (5)
O5	0.0506 (7)	0.0549 (8)	0.0590 (8)	0.0072 (6)	0.0167 (6)	−0.0080 (6)
O6	0.0483 (7)	0.0689 (9)	0.0505 (7)	0.0006 (6)	0.0079 (6)	−0.0046 (6)
C16	0.0547 (10)	0.0395 (9)	0.0449 (9)	−0.0035 (8)	0.0188 (8)	−0.0016 (7)
C12	0.0416 (9)	0.0468 (10)	0.0434 (9)	−0.0064 (7)	0.0151 (7)	0.0038 (7)
C18	0.0481 (9)	0.0477 (10)	0.0437 (9)	−0.0014 (8)	0.0117 (8)	−0.0004 (7)
C14	0.0459 (9)	0.0402 (9)	0.0478 (9)	0.0005 (7)	0.0197 (8)	0.0048 (7)
C11	0.0493 (10)	0.0442 (9)	0.0448 (9)	−0.0058 (8)	0.0189 (8)	−0.0047 (7)
O8	0.0676 (8)	0.0514 (8)	0.0547 (8)	0.0062 (6)	0.0126 (6)	−0.0130 (6)
C10	0.0444 (9)	0.0419 (9)	0.0516 (10)	−0.0010 (7)	0.0210 (8)	0.0019 (7)
C17	0.0733 (13)	0.0658 (13)	0.0511 (11)	0.0015 (10)	0.0139 (10)	−0.0141 (9)
C15	0.0728 (14)	0.0749 (14)	0.0894 (16)	0.0121 (11)	0.0492 (13)	0.0126 (12)
C13	0.0688 (13)	0.0847 (16)	0.0551 (12)	−0.0053 (12)	0.0034 (10)	−0.0148 (11)

Geometric parameters (Å, °)

O1—C1	1.364 (2)	O7—C14	1.391 (2)
O1—H1	0.8200	O7—C15	1.425 (2)
O4—C7	1.372 (2)	O5—C10	1.366 (2)
O4—C8	1.420 (2)	O5—H5	0.8200
O3—C5	1.389 (2)	O6—C12	1.368 (2)
O3—C6	1.431 (2)	O6—C13	1.418 (2)
C2—C3	1.386 (2)	C16—O8	1.367 (2)
C2—C1	1.386 (2)	C16—C18	1.388 (2)
C2—H2	0.9300	C16—C14	1.393 (2)
C3—O2	1.368 (2)	C12—C11	1.386 (2)
C3—C5	1.393 (2)	C12—C14	1.391 (2)
C5—C7	1.388 (2)	C18—C10	1.384 (2)
C7—C9	1.389 (2)	C18—H18	0.9300
O2—C4	1.428 (2)	C11—C10	1.386 (2)
C9—C1	1.388 (2)	C11—H11	0.9300
C9—H9	0.9300	O8—C17	1.423 (2)
C8—H8A	0.9600	C17—H17A	0.9600
C8—H8B	0.9600	C17—H17B	0.9600
C8—H8C	0.9600	C17—H17C	0.9600
C6—H6A	0.9600	C15—H15A	0.9600
C6—H6B	0.9600	C15—H15B	0.9600
C6—H6C	0.9600	C15—H15C	0.9600
C4—H4A	0.9600	C13—H13A	0.9600
C4—H4B	0.9600	C13—H13B	0.9600
C4—H4C	0.9600	C13—H13C	0.9600
C1—O1—H1	109.5	C14—O7—C15	114.37 (14)
C7—O4—C8	116.51 (15)	C10—O5—H5	109.5
C5—O3—C6	113.81 (13)	C12—O6—C13	116.83 (15)
C3—C2—C1	118.89 (16)	O8—C16—C18	124.27 (16)
C3—C2—H2	120.6	O8—C16—C14	115.49 (15)
C1—C2—H2	120.6	C18—C16—C14	120.24 (15)
O2—C3—C2	124.04 (15)	O6—C12—C11	123.91 (15)
O2—C3—C5	115.48 (15)	O6—C12—C14	115.38 (15)

C2—C3—C5	120.48 (15)	C11—C12—C14	120.71 (15)
C7—C5—O3	119.84 (15)	C10—C18—C16	119.19 (16)
C7—C5—C3	119.71 (15)	C10—C18—H18	120.4
O3—C5—C3	120.44 (15)	C16—C18—H18	120.4
O4—C7—C5	115.70 (15)	C12—C14—O7	119.76 (15)
O4—C7—C9	123.82 (15)	C12—C14—C16	119.52 (15)
C5—C7—C9	120.48 (15)	O7—C14—C16	120.71 (15)
C3—O2—C4	117.63 (14)	C10—C11—C12	118.84 (15)
C1—C9—C7	118.82 (15)	C10—C11—H11	120.6
C1—C9—H9	120.6	C12—C11—H11	120.6
C7—C9—H9	120.6	C16—O8—C17	117.52 (14)
O1—C1—C2	116.85 (15)	O5—C10—C18	117.03 (15)
O1—C1—C9	121.55 (15)	O5—C10—C11	121.48 (15)
C2—C1—C9	121.61 (15)	C18—C10—C11	121.49 (16)
O4—C8—H8A	109.5	O8—C17—H17A	109.5
O4—C8—H8B	109.5	O8—C17—H17B	109.5
H8A—C8—H8B	109.5	H17A—C17—H17B	109.5
O4—C8—H8C	109.5	O8—C17—H17C	109.5
H8A—C8—H8C	109.5	H17A—C17—H17C	109.5
H8B—C8—H8C	109.5	H17B—C17—H17C	109.5
O3—C6—H6A	109.5	O7—C15—H15A	109.5
O3—C6—H6B	109.5	O7—C15—H15B	109.5
H6A—C6—H6B	109.5	H15A—C15—H15B	109.5
O3—C6—H6C	109.5	O7—C15—H15C	109.5
H6A—C6—H6C	109.5	H15A—C15—H15C	109.5
H6B—C6—H6C	109.5	H15B—C15—H15C	109.5
O2—C4—H4A	109.5	O6—C13—H13A	109.5
O2—C4—H4B	109.5	O6—C13—H13B	109.5
H4A—C4—H4B	109.5	H13A—C13—H13B	109.5
O2—C4—H4C	109.5	O6—C13—H13C	109.5
H4A—C4—H4C	109.5	H13A—C13—H13C	109.5
H4B—C4—H4C	109.5	H13B—C13—H13C	109.5
C1—C2—C3—O2	−179.75 (15)	C13—O6—C12—C11	4.7 (2)
C1—C2—C3—C5	0.4 (2)	C13—O6—C12—C14	−175.54 (17)
C6—O3—C5—C7	−97.21 (19)	O8—C16—C18—C10	179.30 (16)
C6—O3—C5—C3	83.3 (2)	C14—C16—C18—C10	−0.4 (3)
O2—C3—C5—C7	179.80 (15)	O6—C12—C14—O7	2.6 (2)
C2—C3—C5—C7	−0.3 (2)	C11—C12—C14—O7	−177.60 (14)
O2—C3—C5—O3	−0.7 (2)	O6—C12—C14—C16	−178.57 (15)
C2—C3—C5—O3	179.16 (14)	C11—C12—C14—C16	1.2 (2)
C8—O4—C7—C5	−171.18 (17)	C15—O7—C14—C12	−97.3 (2)
C8—O4—C7—C9	9.5 (3)	C15—O7—C14—C16	83.9 (2)
O3—C5—C7—O4	1.5 (2)	O8—C16—C14—C12	179.76 (15)
C3—C5—C7—O4	−179.02 (15)	C18—C16—C14—C12	−0.5 (2)
O3—C5—C7—C9	−179.10 (14)	O8—C16—C14—O7	−1.5 (2)
C3—C5—C7—C9	0.4 (2)	C18—C16—C14—O7	178.29 (15)
C2—C3—O2—C4	8.9 (2)	O6—C12—C11—C10	178.80 (15)
C5—C3—O2—C4	−171.24 (16)	C14—C12—C11—C10	−0.9 (2)

O4—C7—C9—C1	178.85 (15)	C18—C16—O8—C17	7.3 (3)
C5—C7—C9—C1	−0.5 (2)	C14—C16—O8—C17	−173.01 (16)
C3—C2—C1—O1	179.64 (14)	C16—C18—C10—O5	−178.55 (15)
C3—C2—C1—C9	−0.5 (2)	C16—C18—C10—C11	0.7 (3)
C7—C9—C1—O1	−179.58 (14)	C12—C11—C10—O5	179.19 (15)
C7—C9—C1—C2	0.6 (2)	C12—C11—C10—C18	0.0 (2)

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the C1—C3,C5,C7,C9 and C10—C12,C14,C16,C18 benzene rings, respectively.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O5—H5 \cdots O7 ⁱ	0.82	1.93	2.7484 (18)	179
O1—H1 \cdots O3 ⁱⁱ	0.82	1.90	2.7204 (17)	175
C6—H6A \cdots O1 ⁱⁱⁱ	0.96	2.57	3.256 (3)	129
C15—H15A \cdots O5 ^{iv}	0.96	2.59	3.270 (3)	128
C4—H4B \cdots Cg1 ^v	0.96	2.86	3.777 (2)	160
C17—H17B \cdots Cg2 ^{vi}	0.96	2.85	3.736 (2)	154
C13—H13B \cdots O1 ^{vii}	0.96	2.49	3.303 (3)	142

Symmetry codes: (i) $-x, y+1/2, -z+1/2$; (ii) $-x+1, y-1/2, -z+1/2$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x, -y+2, -z$; (v) $x, -y+1/2, z-1/2$; (vi) $x, -y+1/2, z-3/2$; (vii) $x, -y+3/2, z+1/2$.